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Bloch theorem applied to structures with additional symmetries: reduced unit cell and irreducible Brillouin zone

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Abstract – **Bloch theorem provides a useful tool to analyze wave propagation in periodic systems. While this method has been developed for structures periodic by translation, we show that when glide (translation plus reflection) or screw (translation plus rotation) symmetries are present, they can be accounted by revisiting the boundary conditions of the Bloch theorem. By considering a smaller periodicity, the computational cost decreases and the interpretability of the dispersion diagram improves (i.e. the number of folding and non-interacting intersecting curves is reduced). Concerning computational cost reduction, we recall the choice of the irreducible Brillouin zone in terms of the unit cell symmetries, and we show that band-gap characteristics can not always be obtained from the irreducible Brillouin zone contour, even when the unit cell possesses some symmetries.**

I. Bloch theorem applied to glide and screw symmetric structures: smallest unit cell

Wave propagation in infinite translational periodic structures is often addressed via the Bloch theorem, providing its dispersion characteristics. In a recent work [1], it has been shown that for quasi-one-dimensional wave propagation (one dimensional waves propagating in two or three dimensional structures), glide and screw symmetries can be accounted for, reducing the size of the unit cell. We propose here its generalization to quasi-two-dimensional wave propagation (two dimensional waves propagating in three dimensional structures).

We denote $\boldsymbol{r}_P$ the position of the point P within the reference cell, and by $\boldsymbol{\rho}_P = \boldsymbol{r}_P + n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2$ the same position P relative to the $\{n_1\ n_2\}$-th unit cell, where $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are the basis vectors of the direct lattice. Assuming a harmonic wave with wave vector $\boldsymbol{k}$, the wave displacement $\boldsymbol{u}(\boldsymbol{\rho}_P, t)$ at time t and position $\boldsymbol{\rho}_P$ is given by

$$\boldsymbol{u}(\boldsymbol{\rho}_P, t) = (\mathbf{R_1})^{n_1}(\mathbf{R_2})^{n_2}\boldsymbol{u}(\boldsymbol{r}_P, t)e^{n_1(\boldsymbol{k}\cdot\boldsymbol{e}_1)+n_2(\boldsymbol{k}\cdot\boldsymbol{e}_2)}, \tag{1}$$

where $\mathbf{R_1}$ and $\mathbf{R_2}$ are reflection or rotation matrices. Since there should be no order between the application of the transformation in the $\boldsymbol{e}_1$ or the $\boldsymbol{e}_2$ directions, $\mathbf{R_1}\mathbf{R_2} = \mathbf{R_2}\mathbf{R_1}$. In general two rotation/reflection matrices are noncommutative, meaning that the Bloch theorem can be applied to glide or axisymmetric geometries but not to spherical ones.

We illustrate the advantages of using the smallest symmetry by investigating one-dimensional wave propagation in a longitudinally wrinkled helicoid (twisted and stretched ribbon, see Fig. 1a) [2]. Neglecting the twisting angle, this structure is periodic by translation with period 2λ but is also screw symmetric with period λ (Fig. 1b), and resulting dispersion curves are shown in Fig. 1c and Fig. 1d, respectively. Advantages of using the smallest unit cell are that the computational time is divided by a factor 4 (stiffness and mass matrices grow quadratically), but also resulting dispersion curves are more clear while the provided information is the same. Indeed, the number of folding curves (dashed circles) and non-interacting intersecting curves (dashed squares) is reduced (Figs. 1c-d). Quasi-two-dimensional structures with glide and screw symmetries are also investigated in [3], and are shown in Figs. 1e-g. Moreover, for this last example (Fig. 1g), due to its chiral angle, the nanotube does not possess pure period by translation, such that the classical Bloch theorem cannot be used, whereas the proposed revisited version makes it feasible.

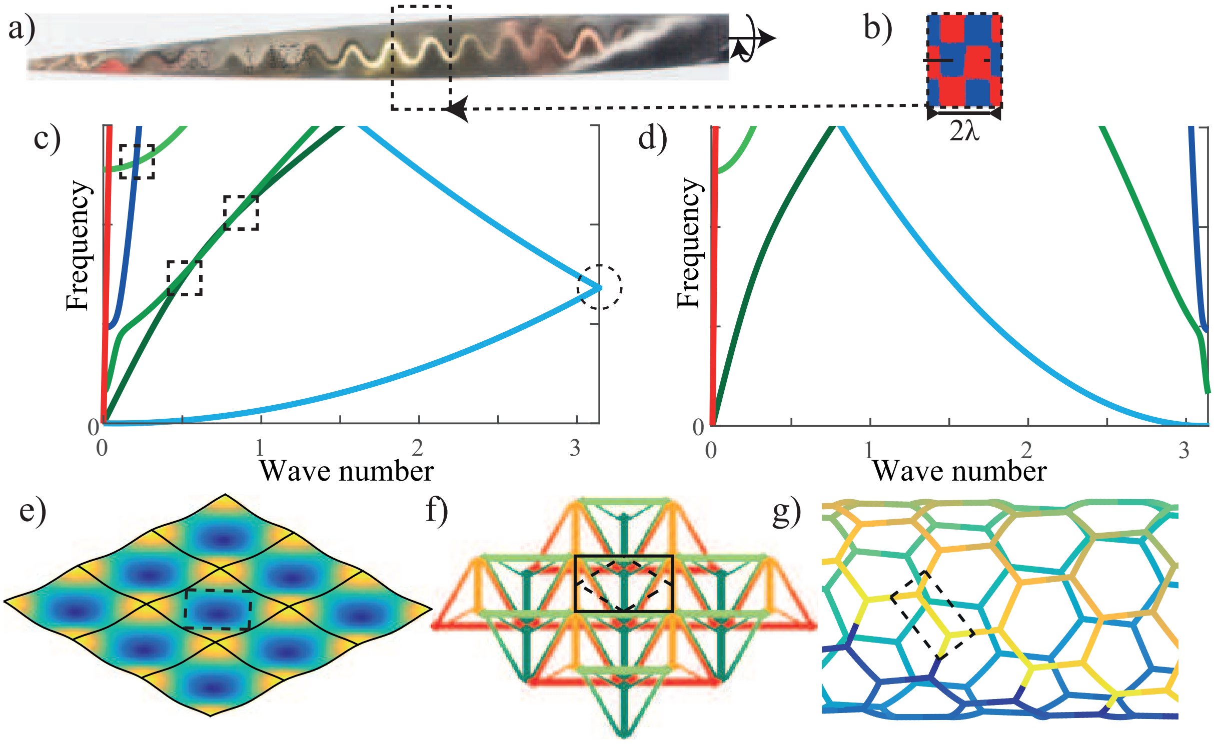

Fig. 1: Longitudinally-wrinkled helicoid (a) and details on its radial stress which is periodic by translation (2λ) and screw periodic (λ). Resulting dispersion curves using the period 2λ (c) and λ (d), where folding and non-interacting intersecting curves are highlighted with dashed circles and squares, respectively. Glide symmetric undulated plate (e) and pyramidal core (f), and screw symmetric nanotube (d), where their translational periods and glide/screw periods are highlighted by full and dashed parallelograms, respectively (e-g).

II. Bloch theorem with symmetric unit cells: irreducible Brillouin zone

It is well established that for time independent harmonic systems, the properties of a wave propagating along an axis does not depend on its sense. For this reason, the maximum irreducible Brillouin zone (IBZ) is half of the first Brillouin zone (FBZ), and can be even reduced when the unit cell possesses some reflection of rotational symmetries, as shown in Fig. 2 (among the 17 different plane crystallographic groups all investigated in [4], only the ones with square unit cells and no pure glide reflection are considered here). However, in the literature of band-gaps, their detection is often restricted to the contour of the IBZ, without justification. To show that this last statement is not accurate, we simulate hundreds of different phononic crystal lattices and sort them by their plane crystallographic groups. For each band-gap detected, the location of its extrema are plotted in Fig. 2.

It is found that for lattices possessing only rotational symmetries (groups p1, p2 and p4), most of the band-gaps extrema are not located at the IBZ contour. Indeed, for such lattices, the IBZ can be arbitrary rotated such that the definition of the contour itself does not really exist. For the other lattices, it is found that the probability that an extremum is located at the IBZ contour increases with the number of reflection axis, but is never 100%. It means that in order to get accurate results, the full IBZ has to be investigated.

III. Conclusion

Metamaterials are often symmetric structures and the correct consideration of the symmetry can drastically reduce the computational cost. In the presence of glide or screw symmetries, the size of the unit cell can be reduced with respect to the translational periodicity, whereas if the cell possesses some reflection symmetries, the size of the irreducible Brillouin-zone contour is restricted to small portions of the the first Brillouin zone. However, although the probability that a band-gap extremum is located at the irreducible Brillouin zone contour increases

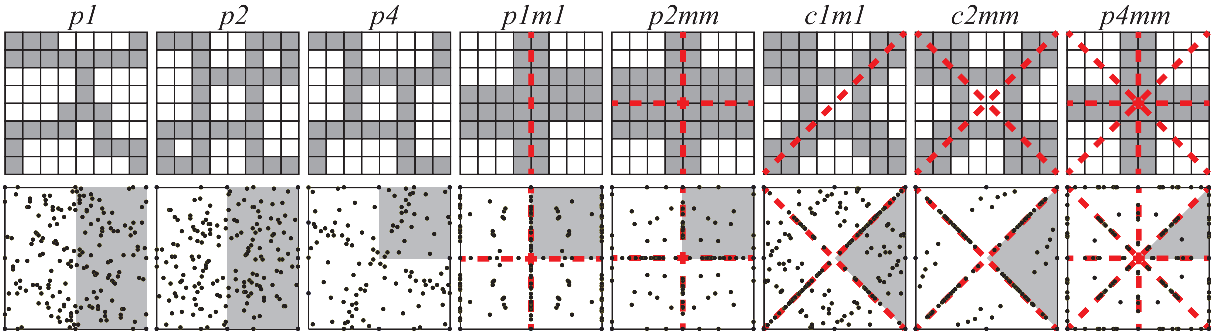

Fig. 2: One example of unit cell for each plane crystallographic group investigated here, and resulting FBZ in the bottom. IBZ in gray and position of the 300 first band-gap extrema in black dots. The red dashed lines indicate mirror axis of the unit cell and in the FBZ. Geometry, material, and mesh details in [4].

with the symmetry order of the lattice, this probability is never 100% and to be sure to get accurate results, the full irreducible Brillouin zone has to be considered.

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